



chain nodes :

6 7 8 9 10 11 12 13 14 15 16 17 24 25 26 27 28 29 30 32 33 34 41 42 48 49

ring nodes :

1 2 3 4 5 18 19 20 21 22 23 31 35 36 37 38 39 40 43 44 45 46 47

chain bonds :

1-6 2-15 4-11 5-7 7-8 8-9 8-10 11-12 11-13 13-14 15-16 15-24 16-17 17-18 24-25
24-32 25-26 26-27 26-34 27-28 27-33 28-29 29-30 30-31 34-35 37-41 39-42 46-48
48-49

ring bonds :

1-2 1-5 2-3 3-4 4-5 18-19 18-23 19-20 20-21 21-22 22-23 31-43 31-47 35-36 35-40
36-37 37-38 38-39 39-40 43-44 44-45 45-46 46-47

exact/norm bonds :

1-2 1-5 1-6 2-3 2-15 3-4 4-5 5-7 7-8 8-10 24-25 24-32 25-26 27-33 28-29 29-30
46-48

exact bonds :

4-11 8-9 11-12 11-13 13-14 15-16 15-24 16-17 17-18 26-27 26-34 27-28 30-31 34-35
37-41 39-42 48-49

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23 31-43 31-47 35-36 35-40 36-37 37-38 38-39
39-40 43-44 44-45 45-46 46-47

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom
32:CLASS 33:CLASS 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:CLASS
42:CLASS 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 49:CLASS